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MODELING OF THE ELASTIC ELECTRONIC POLARIZATION OF L-24 CORDIERITE CERAMIC

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A procedure for modeling the elastic electronic polarization of a specimen of L-24 cordierite ceramic is examined. The results of simulation modeling of the dielectric frequency spectra of oxide crystals of corundum and quartz, which are components of L-24 ceramic, and modeling of a commercial sample of this ceramic are presented.

Key words: elastic electronic polarization, ceramic, cordierite ceramic, dielectric spectrum.

Ordinarily, the conventional procedure of adjusting the composition of ceramics so as to obtain the desired working properties is one step in a multistep technology. Thus, conventional evaluation of the effect of the percentage content of the components on the final characteristics of the prospective sample requires high expenditures of materials, energy and raw-materials resources and time. The current situation can be changed by preliminary mathematical and computer modeling of the characteristics of the desired prototypes. It is evident that the validity of determining the characteristics in the "composition – structure – properties" paradigm which are studied on the basis of calculations are entirely and completely determined by the effectiveness of the mathematical models used.

In turn, cordierite ceramics are being increasingly used in different areas of technology to manufacture electric insulation articles that function in the presence of temperature drops.

Cordierites are solid solutions of magnesium and purely ferruginous substances. The following impurities can be present in such compounds (wt.%): MnO (to 1 – 2%), Fe_2O_3 (to 1 – 1.5%), CaO, K_2O, Na_2O and BeO. In addition, cordierite ceramic contains the following crystalline phases in decreasing amount: mullite, quartz, corundum, magnesium spinel and enstatite.

A number of other crystalline phases are present in this ceramic together with cordierite: mullite ($3Al_2O_3 \cdot 2SiO_2$), corundum, quartz, cristobalite and possibly spinel ($MgO \cdot Al_2O_3$) and magnesium metasilicate ($MgO \cdot SiO_2$). The content of individual crystalline phases depends not only on the initial mass composition but also on a number of technological parameters — the dispersity of the batch components, mass uniformity, firing regime and so forth.

A small amount of a glassy phase formed as a result of the presence of impurities and specially introduced fluxes in the raw materials can be present in cordierite ceramic. A gas phase is also present; its amount is determined by the degree to which the material sinters. The number of pores in the ceramic fluctuates over wide limits from several percents in dense to 15 – 30% in porous material.

The properties of cordierite ceramic are determined by the content of the indicated phases as well as its structure. It should be noted that on the whole the properties of the ceramic improve with increasing cordierite content. Calculations show that depending on the chemical composition of the ceramic its cordierite content fluctuates from 50 – 55% (L-24, K-2 and K-4 ceramic) to 93 – 96% (KDI-2) [1].

We note that because it is present in all, without exception, types of dielectric materials elastic electronic polarization occupies a special place among all the diverse forms of polarization processes. In addition, such processes are least inertial. This makes it possible in the first place to single out explicitly their contribution to the total polarizability of a sample, which greatly simplifies the problem of assessing the adequacy of the fundamental models of the interaction of charged particles with an external electromagnetic field, and in the second place to take account of elastic electronic polarizability as a top priority, which is objectively necessary in order to describe the slower mechanisms.

The mathematical model of elastic electronic polarization of any individual component of an electroceramic consisting of a composition of crystalline oxides can be adequately expressed by a system of equations of forced harmonic oscillations with friction [2, 3].

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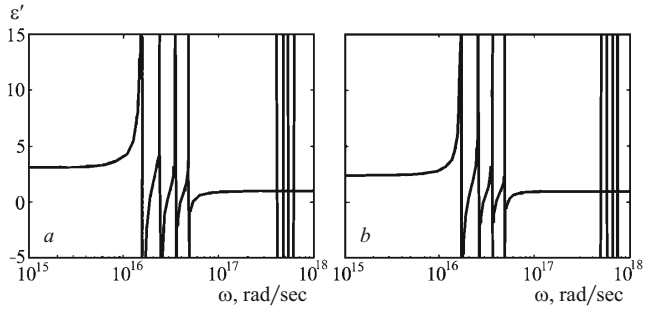

Fig. 1. Computed dielectric spectra of the constituent simple crystals of L-24 ceramic: *a*) ceramic; *b*) quartz.

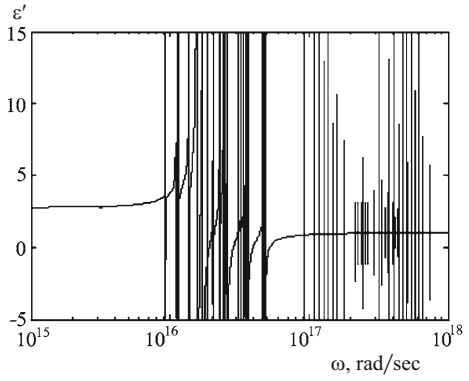

Fig. 2. Computed dielectric spectrum of L-24 corundum ceramic.

The effective charges acting on the internal electrons of an oxygen anion Q_1 as well as all electrons of a cation can be calculated within the framework of Slater's method of linear combination of atomic orbitals. But because of the efficiency with which the parameters of the electronic configuration of the outer (optical) electrons of the ion O^{2-} are determined this basic procedure must be modified [4, 5].

The results of the simulation modeling of the dielectric frequency spectra $\varepsilon'(\omega)$ of oxide crystals of corundum and quartz (Al_2O_3, SiO_2), which are components of L-24 ceramic, are reflected in Fig. 1. The data points represent data obtained from physical measurements of the polarization properties of the experimental crystals.

The results presented show that the model used for the elastic electronic polarization processes in crystalline oxides as well as the method proposed for calculating their dynamic parameters are effective.

Thus, the approach presented here can be used at the applied (engineering) level to predict the operating characteristics of composite dielectrics whose chemical composition is given beforehand.

It is known that the elastic electronic polarization of a simple substance is an additive property, i.e., it is comprised of the polarizabilities of individual ions comprising a formula unit of a particular chemical compound. Thus, a collection of models which describe the deformation of electronic shells and individual particles comprising the experimental sample can be used to study the polarization characteristics of a complex (composite) material [6].

A computational experiment was performed to check how well the frequency spectra of the real part of the complex dielectric constant $\varepsilon'(\omega)$ of a commercial sample of L-24 electrotechnical ceramic is modeled. The results are presented in Fig. 2.

Analysis of the results obtained using the mathematical method to describe the elastic electronic polarization of composite oxide ceramics by comparing the computed values of $\varepsilon'(\omega)$ for the commercial sample studied, which are characteristic for visible-range frequencies, and the control value ε_∞ shows that the structural models presented for the processes studied as well as the method of their parametric synthesis are quite effective.

In summary, the proposed model makes it possible to simulate quite accurately the characteristics of the complex dielectric constant of oxide ceramics in the region where their elastic electronic polarization processes are established. Synthesis of the descriptions proposed was accomplished from the standpoint of the modern systems approach by integrating the fundamental principles of the classical theory of the polarization of dielectrics with the basic principles of the theory of modeling of complex systems as well as using the theory and methods of technical cybernetics.

In turn, bifurcation of the dielectric constant leads to consequent changes of other important parameters of the materials studied, for example, mechanical and electric strength as well as radiation resistance. Therefore, the problem is to find a model that reflects the interrelation of the characteristics of processes occurring in dielectrics under various kinds of actions. Successful implementation of such a mathematical description should make it possible to optimize control of the properties of composite materials by picking the most successful variations of the chemical and component compositions, which evenly affect all their functional qualities, which could result in the development of fundamentally new commercial sample of electroceramics.

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